

# Isophthalic acid, isobutyl 3-methylbut-2-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C17H22O4/c1-12(2)8-9-20-16(18)14-6-5-7-15(10-14)17(19)21-11-13(3)4/h5-8,
<b>InchiKey:</b>	LOOAYZQCMBQKDI-UHFFFAOYSA-N
<b>Formula:</b>	C17H22O4
<b>SMILES:</b>	CC(C)=CCOC(=O)c1cccc(C(=O)OCC(C)C)c1
<b>Mol. weight [g/mol]:</b>	290.35

## Physical Properties

Property code	Value	Unit	Source
gf	-203.57	kJ/mol	Joback Method
hf	-556.60	kJ/mol	Joback Method
hfus	34.38	kJ/mol	Joback Method
hvap	74.34	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.622		Crippen Method
mcvol	237.210	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	2182.00		NIST Webbook
tb	776.20	K	Joback Method
tc	987.88	K	Joback Method
tf	430.57	K	Joback Method
vc	0.902	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.54	J/mol×K	776.20	Joback Method
cpg	694.83	J/mol×K	811.48	Joback Method
cpg	709.08	J/mol×K	846.76	Joback Method
cpg	722.30	J/mol×K	882.04	Joback Method
cpg	734.55	J/mol×K	917.32	Joback Method
cpg	745.83	J/mol×K	952.60	Joback Method
cpg	756.18	J/mol×K	987.88	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U343934&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343934&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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